

Chloralose

15879-93-3 | DTXSID4020088

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 177 °C

Global applicability domain: Inside

Local applicability domain index: 3.05e-01

Confidence level: 5.98e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Chloralose</div> <div>Measured: 183</div> <div>Predicted: 177</div>	<div>Image not found</div> <div>Urochloralic acid</div> <div>Measured: 142</div> <div>Predicted: 141</div>	<div>Image not found</div> <div>Isopropyl beta-D-1-thiogalactopyranoside</div> <div>Measured: 121</div> <div>Predicted: 132</div>
<div>Image not found</div> <div>Ascorbyl palmitate</div> <div>Measured: 117</div> <div>Predicted: 113</div>		